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THERMAL NEUTRON SPECTRA IN UNIFORM LATTICES • USE OF CADILHAC'S FORMALISM

by

P. HAUBERT
(BelgoNucléaire)

1967

EURATOM/US Agreement for Cooperation

EURAEC Report No. 1814 prepared by BelgoNucléaire,
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In heterogeneous systems such as the unit cell of a uniform lattice, the fine structure of the flux can very often be evaluated at each energy by mono-energetic transport or diffusion theory. For instance, the method of Amouyal and Benoist uses integral transport theory in the fuel region and adjusted diffusion theory in the moderator. This method can be generalized by the determination of the flux in the fuel element, cladding included, with the help of collision probabilities in annular systems; the use of diffusion theory in the moderator region can also be avoided. Once the fine structure has been determined, effective cross-sections can be defined and the treatment of thermalization in these systems can be done in exactly the same way as in homogeneous systems.

In some cases such energy space separation is no longer possible, for instance when the unit cell has several distinct thermalizing regions. Cadilhac's model can still be used easily when the number of thermalizing regions is small, but the complexity of the computational scheme increases rapidly with the number of such regions.

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- R E S U M E -

Ce rapport traite de l'utilisation du modèle synthétique de thermalisation proposé par Cadilhac pour la détermination des flux neutroniques dans des systèmes homogènes et hétérogènes et plus particulièrement dans la cellule élémentaire d'un réseau uniforme.

Dans des systèmes homogènes, le flux neutronique et la densité de ralentissement obéissent à deux équations différentielles couplées régissant la conservation et la thermalisation des neutrons respectivement. Le flux neutronique peut être calculé de différentes façons, par exemple en transformant le système d'équations en deux équations différentielles du premier ordre, ou en une équation de Shrödinger, ou encore en une équation de Riccati suivie d'une intégration simple.

Dans des systèmes hétérogènes, tels que la cellule élémentaire d'un réseau uniforme, la structure fine du flux peut souvent être définie à chaque énergie à l'aide de la théorie monocinétique du transport ou de la diffusion. La méthode d'Amouyal et Benoist, par exemple, repose sur la théorie intégrale du transport dans la région combustible et sur la théorie asymptotique de diffusion dans le modérateur. Cette méthode peut être généralisée par l'emploi de probabilités de collision en géométrie cylindrique pour le calcul du flux dans l'élément combustible, gaine comprise ; il est également possible d'éviter le recours à la théorie de diffusion dans le modérateur. Quand la structure fine du flux a été calculée, on peut définir des sections efficaces, effectives et poursuivre le traitement de la thermalisation dans ces systèmes, exactement de la même façon que dans les systèmes homogènes.

Dans certains cas, la séparation des variables énergétique et spatiale n'est pas possible, comme par exemple quand la cellule élémentaire contient plusieurs régions thermalisantes distinctes. Le modèle de Cadilhac peut encore être d'un emploi aisé quand le nombre de régions thermalisantes est faible, mais le schéma de calcul augmente rapidement en complexité avec le nombre de ces régions.

* * *

- F O R E W O R D -

The work described in this paper was launched by BelgoNucléaire in 1963 as an attempt to define a basic formalism to be applied in the PANTHER code. Its assessment to graphite lattices was part of commitment from DRAGON (contract CON/WIN/57006). The application to UO_2 - PuO_2 - H_2O systems has been performed in the scope of the shared contract Euratom-C.E.N. - BelgoNucléaire (contract 001-64-1 TRUB).

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1.- INTRODUCTION.

The neutron flux in a heterogeneous system is given as the solution of Boltzmann's transport equation :

$$\left[\frac{1}{v} \frac{\partial}{\partial t} + \bar{\Omega} \cdot \bar{\nabla} + \Sigma (\bar{r},E) \right] \Phi (\bar{r},E,\bar{\Omega},t) = \varkappa(\bar{r},E,\bar{\Omega},t) \qquad (1)$$

where the emission density $\varkappa$ is given by :

$$\varkappa (\bar{r},E,\bar{\Omega},t) = \int d\bar{\Omega}' \int dE' \left[\Sigma_s(\bar{r},E' \rightarrow E,\mu_o) \Phi (\bar{r},E',\bar{\Omega}',t) \right] + S(\bar{r},E,\bar{\Omega},t)$$

with $\mu_o = \bar{\Omega} \cdot \bar{\Omega}'$

$\Sigma (\bar{r},E)$ is the total macroscopic cross section at the energy E,

$\Sigma_s(\bar{r},E' \rightarrow E,\mu_o)$ is the transfer macroscopic cross section from energy E' to energy E, from direction $\bar{\Omega}'$ to direction $\bar{\Omega}$,

$\Phi (\bar{r},E,\bar{\Omega},t)\, dE$ is the flux of neutrons with energies between E and E + dE at point $\bar{r}$ in the direction $\bar{\Omega}$ and at time t,

$S (\bar{r},E,\bar{\Omega},t)$ is the external source density.

Adequate numerical methods have been proposed by combining the multigroup approximation and P_N or S_N transport methods but they lead to excessive running times for routine calculations.

In the stationary case, with no external sources, and assuming an isotropic emission density, the transport equation can be written in the integral form :

$$\Phi(\bar{r},E) = \int dV \left[\varkappa(\bar{r},E) \cdot \frac{1}{4\pi \mid \bar{r} - \bar{r}' \mid^2} \exp\left(- \int_{\bar{r}'}^{\bar{r}} \Sigma \, ds \right) \right] \qquad (1')$$

$\Phi(\bar{r},E)$ is the scalar flux and $\varkappa(\bar{r},E)$ the isotropic emission density.

If the system can be divided in N homogeneous regions where the flux can be considered as constant, the relation (1') can be replaced by the N relations

$$\Phi_j(E) = \sum_{i=1}^{N} \frac{P_{j,i}(E)}{\Sigma_i(E)} \varkappa_i(E) \qquad j = 1,N \qquad (2)$$

Φ_j and $\varkappa_j$ are the volume averaged flux and emission density and Σ_j the total cross section in zone j. $P_{j,i}(E)$ is the probability that a neutron uniformly and isotropically born in zone j, collides for the first time in zone i :

$$P_{j,i}(E) = \frac{\Sigma_i(E)}{V_j} \int\int \frac{\exp\left(- \int_{\bar{r}_i}^{\bar{r}_j} \Sigma \, ds \right)}{4\pi \mid \bar{r}_i - \bar{r}_j \mid^2} dV_i \, dV_j \qquad (3)$$

where r_i denotes a point in zone i and r_j a point in zone j.

The reciprocity relation is an immediate consequence of this expression and reads :

$$\Sigma_i \, P_{i,j} \, V_i = \Sigma_j \, P_{j,i} \, V_j \qquad (4)$$

Introducing the slowing-down density q(E) defined as the difference between the number of neutrons down-scattered from an energy higher than E to an energy lower than E and the number of neutrons crossing E in the opposite direction, the emission density can be written :

$$\varkappa(\bar{r},E) = \int_0^\infty dE'\ \Sigma_s(\bar{r},E' \to E)\ \Phi(\bar{r},E')$$

$$= \Sigma_s(\bar{r},E)\ \Phi(\bar{r},E) + \frac{\partial\, q(\bar{r},E)}{\partial\, E} \qquad (5)$$

The study of neutron thermalization will establish a relation between the slowing-down density q and the neutron flux Φ , whereas the study of the geometrical heterogeneity will define the collision probabilities. The fundamental equations to be solved are :

$$\Sigma_j\ \Phi_j\ V_j = \sum_{i=1}^{N} P_{i,j}\ \varkappa_i\ V_i \qquad j = 1,N \qquad (6)$$

*

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2.- TREATMENT OF THERMALIZATION.

2.1. THE CADILHAC'S MODEL.

Let us consider, in an infinite homogeneous system, the function :

$$C(E) = \frac{d}{dE}\left(\frac{\Phi(E)}{M(E)}\right)$$

M(E) being the Maxwellian flux at the temperature T of the system and K the Boltzmann constant.

$$M(E) = \frac{E}{(KT)^2}\exp\left(-\frac{E}{KT}\right)$$

The flux being Maxwellian in an infinite non absorbing medium, the function C(E) can be interpreted as the departure, due to the absorptions, of the neutron distribution from the equilibrium Maxwellian spectrum. By using the principle of detailed balance, q is related to C by an integral Hermitian operator. The idea of Cadilhac was to consider the inverse operator J [1] :

$$C \equiv \frac{d}{dE}\left(\frac{\Phi(E)}{M(E)}\right) = J\,q(E) \qquad (7)$$

J is an Hermitian positive definite operator. In the synthetic model proposed by M. Cadilhac one considers that J is a differential second order operator. As it is self-adjoint it is written :

$$J(E) = j(E) - \frac{d}{dE}\left(k(E) \frac{d}{dE} \right) \qquad (7')$$

This form of J is shown to be rigorous in two extreme cases : the monoatomic hydrogeneous gas and the heavy free gas, and it can represent with a very good approximation all usual moderators.

In the "Generalized Heavy Free Gas" model of Horowitz the operator J(E) reduces to :

$$J(E) = j(E) \qquad (7'')$$

This is called the primary model.

In the secondary model, j(E) and k(E) are non zero functions related to the scattering law $S(\alpha,\beta)$ of the system. The relation however is not univocal and J.L. Soulé [2] has studied the best way to adjust j and k on the physical model. In order to take into account the asymptotic behaviour of j(E) and k(E) at high energies, two new functions are introduced :

$$\left.\begin{aligned} H(E) &= \xi\, \Sigma_s(\infty) \,.\, M(E) \,.\, k(E) \\ G(E) &= \xi\, \Sigma_s(\infty) \,.\, M(E) \,.\, EKT \,.\, j(E) \end{aligned}\right\} \qquad (8)$$

For high values of E, G and H have finite limits , besides, the relation between Φ and q becomes :

$$\Phi(E) = \frac{1}{\xi\, \Sigma_s(\infty)} \left[G(E) \frac{q(E)}{E} - H(E) \frac{dq(E)}{dE} \right] \qquad (9)$$

This is the fundamental equation of the classical Greuling - Goertzel model of neutron slowing-down in the epithermal range. It includes :

- the continuous slowing-down model of Fermi corresponding to $H(E) = 0$,
- the model of Selengut - Goertzel for the monoatomic hydrogeneous gas corresponding to $H(E) \equiv 1.0$, $G(E) \equiv 1.0$.

2.2. ALTERNATIVE FORMS OF THE FLUX EQUATIONS.

The system of equations describing the flux in an infinite homogeneous medium :

$$-\frac{dq}{dE} = \Sigma_a \Phi \tag{10}$$

$$\frac{d}{dt}\left(\frac{\Phi}{M}\right) = \Sigma_a q - \frac{d}{dE}\left(k \frac{dq}{dE}\right) \tag{11}$$

or

$$EKT \frac{d\Phi}{dE} + (E - KT)\,\Phi = \frac{G}{\xi \Sigma_s} q - EKTM \frac{d}{dE}\left(k \frac{dq}{dE}\right) \tag{11'}$$

is amenable to a variety of treatments.

In particular Cadilhac has shown [3] that it can be advantageous to replace (11) by an equivalent expression :

$$\frac{d}{dE}\left(\frac{\Phi}{M}\right) = \Sigma_o q - \frac{1}{q_o} \frac{d}{dE}\left[k q_o^2 \frac{d}{dE}\left(\frac{q}{q_o}\right)\right] \tag{12}$$

with $$q_o(E) = \int_0^E \frac{1}{\sqrt{E}} M(E)\, dE$$

$$j_o(E) = j(E) - \frac{1}{q_o} \frac{d}{dE} \left(k \frac{dq_o}{dE} \right) \qquad (13)$$

When the absorption of the system is moderate and mostly 1/v, $\frac{q}{q_o}$ is a very slowly varying function and the first term of the RHS of (12) is predominant. In this case, one has a very good first approximation by ignoring the second term ; equation (12) reduces then to its form with the primary model. Moreover the function

$$G_o(E) = \xi \Sigma_s M(E) \cdot EKT \cdot j_o(E)$$

behaves generally better than G, especially at low energies ; at high energies, however, both functions are equal, q_o being practically constant and little is gained by going to (12), particularly when $\Sigma_a(E)$ presents strong resonances.

At high energies ($E/KT \geq 3$) it seems more interesting to define an auxiliary variable U(E) by :

$$U(E) = \Phi(E) \left(1 + \frac{H \Sigma_a}{\xi \Sigma_s} \right) \qquad (14)$$

The system of equations (10) and (11) can then be transformed into :

$$\left.\begin{aligned} \frac{dq}{dE} &= \Sigma_a^*(E)\, U(E) \\ \frac{d}{dE}\ \frac{U}{M} &= J(E)\, q(E) \end{aligned}\right\} \qquad (15)$$

$$\text{with} \qquad \Sigma_a^*(E) = \Sigma_a(E)\left(1 + \frac{H\,\Sigma_a}{\xi\,\Sigma_s}\right)^{-1} \qquad (16)$$

This system is formally similar to that obtained with the primary model, thus, the use of the secondary model entails no additional difficulties. The advantage of this formalism is that $\Sigma_a^*(E)$ and $U(E)$ are smoother than $\Sigma_a(E)$ and $\Phi(E)$, especially at epithermal energies where $\Sigma_a(E)$ can present strong resonances, particularly in plutonium loaded systems.

The system of equation (15) can be transformed into

$$\frac{dq}{dE} = \Sigma_a^*\, U \qquad (17')$$

$$\xi\,\Sigma_s\ \frac{d}{dE}\left\{\frac{1}{G(E)}\left[\ EKT\ \frac{dU}{dE} + (E - KT)\ U\ \right]\right\} = \Sigma_a^*\, U \qquad (17'')$$

where the second equation can be solved independently.

For instance the finite difference scheme of Spectrox [4] can be used ; this scheme is very fast and can be easily extended to heterogeneous systems (when the number of regions is small), but its accuracy is poor.

Instead of equation (17") one could also obtain a second order differential equation in q :

$$\frac{d}{dE}\left[\frac{1}{\Sigma_a^* M}\frac{dq}{dE}\right] = Jq \qquad (18)$$

Equations (17") and (19) can be transformed into first order Riccati equations. For example by introducing the new variable :

$$w = \frac{1}{\xi \Sigma_s}\cdot\frac{1}{J}\cdot\frac{1}{U}\frac{d}{dE}\left(\frac{U}{M}\right)$$

$$= \frac{1}{G}\left[EKT\frac{1}{U}\frac{dU}{dE} + (E - KT)\right] \qquad (19)$$

equation (17") becomes :

$$\frac{dw}{dE} = \frac{\Sigma_a^*}{\xi \Sigma_s} + \left(\frac{1}{KT} - \frac{1}{E}\right)w - \frac{G}{EKT}w^2 \qquad (20)$$

The advantage of this formulation would be to allow to evaluate first w by a first order differential equation, and then the flux by integration of (19) giving immediately :

$$\Phi = \frac{U}{1 + \frac{H\Sigma_a}{\xi\Sigma_s}} = \frac{E}{1 + \frac{H\Sigma_a}{\xi\Sigma_s}} \exp\left\{-\frac{E}{KT} + \int_0^E \frac{G}{EKT} w\, dE\right\} \qquad (21)$$

instead of having to solve a second order differential equation or two coupled first order differential equations. w is a measure of the departure of the flux from the equilibrium Maxwellian spectrum and it is thus a slowly varying function at low energies, except for the factor 1/G. This factor could anyhow be taken out of the definition of the variable by writing :

$$v = EKT \frac{U'}{U} + (E - KT) \qquad (19')$$

Equation (20) then becomes :

$$\frac{dv}{dE} = G \frac{\Sigma_a^*}{\xi \Sigma_s} + \left(\frac{G'}{G} + \frac{1}{KT} - \frac{1}{E} \right) v - \frac{1}{EKT} v^2 \qquad (20')$$

with the disadvantage of having to differentiate G, generally given in a tabulated form. It is interesting to note that although the flux is far from being Maxwellian in the epithermal range, w and v still have a rather smooth variation. Indeed for a 1/E flux, one has :

$$v = E - 2KT$$

Equation (18) can be transformed in a similar way ; by posing :

$$R = \frac{1}{\Sigma_a^*} \frac{1}{q} \frac{dq}{dE} \qquad (22)$$

one gets :

$$R' = \frac{G}{\xi \Sigma_s} \frac{1}{EKT} + \left(\frac{1}{KT} - \frac{1}{E} \right) R - \Sigma_a^* R^2 \qquad (23)$$

The flux is now expressed by :

$$\Phi = \frac{1}{\left(1 + \frac{(H \Sigma_a)}{\xi \Sigma_s} \right)} Rq$$

As a matter of fact, the Riccati equations can only be used with homogeneous systems or more generally with systems having only one thermalizing region. The Sofocate code [5] and its updated version, Leopard, solve a particular form of the Riccati equation corresponding to the Wigner - Wilkins equation.

For some applications it is very interesting to transform equation (17") into a Shrödinger equation. This can be done by introducing a new variable :

$$\phi = U \frac{1}{\sqrt{G}} \exp\left(+ \frac{E}{2KT} \right) \tag{24}$$

ϕ obeys the Shrödinger equation

$$\phi'' + S\,\phi = 0 \tag{25}$$

with

$$S = - \frac{G}{EKT} \frac{\Sigma_a^*}{\xi\,\Sigma_s} + \frac{1}{2} \frac{G''}{G} - \frac{3}{4} \left(\frac{G'}{G} \right)^2 + \frac{G'}{G} \left(\frac{1}{E} - \frac{1}{2KT} \right)$$

$$+ \frac{1}{EKT} - \frac{1}{4(KT)^2} \tag{26}$$

Corngold [6] had already shown all the use that can be made of such an expression in the particular cases of the Wigner - Wilkins and Wikins models. Williams [7] extended his treatment to the secondary model and showed how one can evaluate time and space eigenvalues by the W.K.B. methods without solving explicitly equation (25).

From the computationnal point of vue, the Shrödinger form of the flux equation could seem interesting since very fast methods are available for the solution of equations of this type, as well for boundary value problems as for initial value problems.

However, particular attention should be paid to the behaviour of ϕ and G at very low energies ; in the general case ϕ behaves as $E^{3/4}$ and G as E^{-2} in the vicinity of zero energy. Two other facts decrease the attractiveness of equation (25) for numerical computation:

- at epithermal energies ϕ grows quasi exponentially as exp (E/2KT),
- all oscillations in G (and there are some oscillations for usual moderators) are automatically reflected in the dependent variable ϕ , whereas the dependent variables of other forms of the flux equation are relatively insensitive to the behaviour of G(E), at least for moderate absorption.

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3.- TREATMENT OF HETEROGENEITY.

3.1. POSITION OF THE PROBLEM.

We shall restrict ourselves in the following to a two dimensional lattice but the synthetic model of thermalization can certainly be used in relation which any form of heterogeneity. The system will be considered as infinite in the third dimension and the elementary cell will consist in N successive regions N_i, as shown in figure 1. All boundaries between regions are circular except for the outer boundary of the outermost regions, which is square or hexagonal. The collision probability $P_{i,k}$ can be considered as the probability that a neutron born in V_i, or any of its images V_i^m in the lattice, will undergo its next collision in V_k :

$$P_{i,k} = P^{o}_{i,k} + \underset{m \geq i}{\text{Sum}} P^{m}_{i,k} \qquad (27)$$

where $P^{o}_{i,k}$ is the probability of collision in V_k for a neutron born in the region V_i of the same cell, while $P^{m}_{i,k}$ to the same probability but for neutrons born in any image V_i^m of V_i.

In a system such as that of figure 1, the probabilities $P^{o}_{i,k}$ for i and k smaller than N, N being the index of the outermost region, are relatively easy to evaluate, the system being one dimensional. The other probabilities are more troublesome, since they should be evaluated in two dimensional geometry. Two different cases are to be considered according to the characteristics of the outermost region.

1. The outermost region is large and weakly absorbing, as for most graphite and heavy water moderated systems where this region is the moderating region. In this case diffusion theory is applicable in region V_M and the outer boundary of the cell can be circularized without loss of accuracy. This is the basis of the method of Amouyal and Benoist (generally referred to as the ABH method) and of the Spectrox method.

2. If region V_M is not such that diffusion theory is applicable, its outer boundary can still be circularized, provided that a proper boundary condition can be found. It seems that the condition of isotropic boundary flux used in various codes [8] , [9] and [10] , is adequate. Sauer [11] pointed out that such an approximation can be avoided by the use of the Dancoff correct on C and he presented a scheme for the evaluation of C in the actual geometry of the lattice. As the final formalism for the determination of the fluxes (but not of the probabilities) is the same as in the approximation of isotropic boundary flux, we shall only consider the use of the synthetic model of thermalization with the latter method.

3.2. TREATMENT OF HETEROGENEITY WITH A LARGE, WEAKLY ABSORBING, OUTER REGION.

3.2.1. General formulation.

Let L = N-1 be the number of regions, where the flux can be considered as uniform, besides the external outer region. As this latter region is generally the moderating region, it will be identified by the index M. The fundamental equation (6) can not be written :

$$\Sigma_j V_j \phi_j = \sum_{i=1}^{L} P^{o}_{i,j} \varkappa_i V_i + S_L J^{-}_L P_{b,j} \qquad j = 1,L \qquad (28)$$

where J_L^- is the inward current per unit area at the moderator inner surface S_L and $P_{b,j}$ the probability for a neutron crossing the moderator inner surface, according to a given angular distribution, to collide for the first time in V_i.

Besides the L fundamental equation (28), the conservation equation in the moderator :

$$\left(\varkappa_M - \Sigma_{s,M}\, \Phi_M \right) V_M = \Sigma_{a,M}\, V_M\, \Phi_M + S_L\, j_L(E) \qquad (29)$$

and the global conservation equation in the inner regions :

$$\sum_{k=1}^{N} \Sigma_{a,k}\, V_k\, \Phi_k - \sum_{k=1}^{N} \left(\varkappa_k - \Sigma_{s,k}\, \Phi_k \right) V_k = S_L\, j_L \qquad (30)$$

a further relation between j_L , j_L^- and Φ_M is needed for the evaluation of the L + 3 unknowns Φ_i (i = 1, 2, ..., L), Φ_M , j_L and j_L^-.

This relation will be provided by the diffusion theory applied to the flux in the moderator. Horowitz and Tretiakoff [3] have studied the flux in the moderator in terms of buckling eigenfunctions and they have shown that, with a very good approximation :

$$\Phi_M(E) = \Phi\,(r_L, E) \left[1 + \frac{r_L}{\Lambda}\, h\left(\frac{r_M}{r_L} \right) \right] \qquad (31)$$

where r_L and r_M are the inner and outer radii of the external moderator region respectively, Λ the extrapolation distance at the inner surface and :

$$h(y) = \frac{y^2}{y^2 - 1}\left[\frac{y^2}{y^2 - 1}\ln y - \frac{3}{4} + \frac{1}{4y^2}\right] \qquad (32)$$

The underlying assumptions are, besides the treatment of moderator by diffusion approximation, the boundary conditions :

$$\left.\begin{aligned} &\frac{d\Phi}{dr}\left(r = r_M\right) = 0 \\ &\frac{d\Phi}{dr}\left(r = r_L\right) = \frac{1}{\Lambda}\,\Phi\,(r_L) \end{aligned}\right\} \qquad (33)$$

A relation between j_L and j_L^- is provided either by the diffusion theory or by the blackness concept ; both lead to :

$$j_L^- = \frac{3}{4}\left(\Lambda\,\Sigma_{tr,M} + \Gamma\right) j_L \qquad (34)$$

with $\Gamma = 2/3$ in diffusion theory (35)

$= \Gamma\left(r_L\,\Sigma_{tr,M}\right)$ in Kushneriuk's method for a grey body

$= \frac{4}{3} - \lambda_{bb}$ in Amouyal - Benoist's method [12]; λ_{bb} is the extrapolation length of a black body in an infinite medium.

With the help of Fick's law Λ can be eliminated from (34) the desired supplementary equation is eventually found to be :

$$j_L^-(E) = \frac{1}{4}\,\Phi_M(E) + \left[\frac{3}{4}\,\Gamma\,(E) - \frac{r_L}{4\,D_M}\,h\left(\frac{r_M}{r_L}\right)\right] j_L$$

$$= \frac{1}{4}\,\Phi_M(E) + X'\,j_L \qquad (36)$$

Equations (28) , (29) and (30) still contain the variable $\varkappa_i$ which by averaging of (5), can be expressed as :

$$\varkappa_i(E) = \Sigma_{s,i}(E)\ \Phi_i(E) + \frac{dq_i(E)}{dE}$$

The slowing-down densities are related to the fluxes by the thermalization equations in each region :

$$\frac{d}{dE}\left(\frac{\Phi_i(E)}{M_i(E)}\right) = j_i(E)\ q_i(E) - \frac{d}{dE}\left(k_i(E)\ \frac{dq_i(E)}{dE}\right) \qquad (37)$$

$$i = 1,N$$

$M_i(E)$ being the Maxwellian flux at the mean temperature of zone i.

Hence the system of equations describing the spatio-energetic distribution of the flux in the unit cell of the lattice is made up of the 2L + 4 equations (28) , (29) , (30) , (36) and (37) in the 2L + 4 unknown quantities Φ_i , q_i (i=1,L) , Φ_M , q_M , j_L and $\vec{j}_L \cdot \vec{j}_L$ is easily eliminated with the help of relation (36).

3.2.2. The three regions cell.

The fundamental system of equations is relatively easy to solve on a computer. However, for a large class of reactors, the unit cell consists in a central fuel region, surrounded by a can and possibly a gap, and an external moderator.

For such systems where the can is absent or may be neglected, Amouyal and Benoist, and later Leslie, have developped very fast methods. We shall see in the next section how these methods can be extended to a usual fuel element.

Let r_1 , r_2 and r_3 be the outer radii of the fuel, gap and moderator regions respectively. Following Newmarch's analysis [13], but using the blackness concept the current of neutrons entering the rod per unit length is found to be

$$J_1^- = 2 \pi r_1 j_1^- = \frac{\pi}{2} r_1 \Phi_M + X J_1 \qquad (36')$$

where $J_1 = J_2$ is the net current for unit length and

$$X = \frac{3}{4} \Gamma n\left(\frac{r_1}{r_2} \right) - \frac{r_1}{4 D_M} h\left(\frac{r_3}{r_2} \right) \qquad (38)$$

With Newmarch's assumption of linear anisotropy the expression for $n(r_1/r_2)$ is :

$$n\left(\frac{r_1}{r_2} \right) = \frac{2}{\pi} \left\{ \arcsin \frac{r_1}{r_2} + \frac{r_1}{r_2} \left[1 - \left(\frac{r_1}{r_2} \right)^2 \right]^{1/2} \right\} \qquad (39)$$

while Amouyal and Benoist find, with the assumption of isotropy :

$$n\left(\frac{r_1}{r_2} \right) = \frac{r_1}{r_2} \qquad (39')$$

If the optical thickness of the fuel region is small ($\Sigma_1 r_1 < 1$), the self collision probability $P^o_{1,1}$ can be evaluated with the assumption of spatially uniform flux and it has been tabulated by Case and a al. [14] as $P_c(\Sigma_1 r_1)$. On the other hand the probability of collin the fuel for a neutron hitting its surface with an isotropic angular distribution is readily given by the reciprocity relation :

$$P'_{b,1} = 2 r_1 \Sigma_1 \left(1 - P^o_{1,1} (r_1 \Sigma_1) \right) \qquad (40)$$

The fundamental system of equations can then be rewritten :

$$\begin{aligned}
&\Sigma_1 V_1 \Phi_1 = P^o_{1,1} \varkappa_1 V_1 + P'_{b,1} J^-_1 && (a)\\
&V_M L_M \Phi_M = \Sigma_{a,M} \Phi_M V_M + J_1 && (b)\\
&V_1 L_1 \Phi_1 = \Sigma_{a,1} \Phi_1 V_1 - J_1 && (c)\\
&J^-_1 = \frac{\pi}{2} r_1 \Phi_M + X J_1 && (d)
\end{aligned} \qquad (41)$$

The gap need not, of course, be explicitly considered but it is taken into account for the evaluation of J^-_1 . $P'_{b,1}$ should not be mistaken for $P_{b,1}$ to which it is related by :

$$P'_{b,1} = \frac{r_2}{r_1} P_{b,1}$$

When the optical thickness of the fuel region is not small ($\Sigma_1 r_1 > 1$) the division of this region into numerous homogeneous subregions can be avoided by considering the successive collision probabilities P_k in region 1for a neutron entering the rod with an isotropic angular distribution. Let us consider for a while the case of a non thermalizing fuel region. Equation (41a) can then be written :

$$\Sigma_{a,1} V_1 \Phi_1 = \beta_1 J^-_1 \qquad (42)$$

The quantity

$$\beta_1 = \frac{\Sigma_{a,1} V_1 \Phi_1}{J^-_1} = \frac{J_1}{J^-_1} \qquad (43)$$

is called the blackness of the rod. For a non thermalizing rod and $\Sigma_1 r_1 < 1$, it is given by :

$$\beta_1 = \frac{(1 - C_1) P'_{b,1}}{1 - C_1 P^o_{1,1}} \qquad (44)$$

with

$$C_1 = \frac{\Sigma_{s,1}}{\Sigma_1}$$

The success of the method of Amouyal and Benoist rests on the facility with which β_1 can still be evaluated for $\Sigma_1 r_1 > 1$; it is then given by

$$\beta_1 = P_o(1 - C_1) + P_o P_1 C_1(1 - C_1) + P_o C_1 P_1 P_2(1 - C_1) + \cdots$$

$$= P_o(1 - C_1) \left[1 + P_1 C_1 + P_1 P_2 C_1^2 + \cdots \right] \qquad (45)$$

with $P_o = P'_{b,1}$

In the flat flux approximation all P_i ($i \geq 1$) are considered equal to $P^o_{1,1}$ and one finds (44). Amouyal and Benoist have considered the probability

$$P = \frac{\beta_1}{2 r_1 \Sigma_{a,1}}$$

and have found that, provided that C_1 and $\Sigma_1 r_1$ are not too large

$$\frac{1}{P} \approx 1 + r_1 \Sigma_{a1} + A(1 - C_1)(1 + \alpha_1 C_1 + \alpha_2 C_1^2) \tag{46}$$

where A , α_1 and α_2 are functions of $\Sigma_1 r_1$ only. In particular

$$A = \frac{P^o_{1,1}}{1 - P^o_{1,1}} - r_1 \Sigma_1 \tag{47}$$

Leslie has tried to extend the method of Amouyal and Benoist to systems where the fuel region is thermalizing; in this formalism, equation (41a) is now to be replaced by

$$\left(\frac{1}{S} - Rz \right) \Sigma_1 V_1 \Phi_1 = J_1^- \tag{48}$$

with

$$z = \left(L_1 - \Sigma_{a,1} \right) \frac{1}{\Sigma_1}$$

$$S = P_o \left(1 + P_1 + P_1 P_2 + \cdots \right)$$

$$R = \frac{P_o}{S^2} \left(P_1 + 2 P_1 P_2 + \cdots \right) \tag{49}$$

Equation (48) has been deduced under the assumption that the operator z is weak (i.e. that $z(\Sigma_1 V_1 \Phi_1) << \Sigma_1 V_1 \Phi_1$) and that either all P_i ($i \geq 1$) are equal or z can be permuted with P . Its validity has been checked [15] in the particular case of a non thermalizing fuel region. Then z reduces to the scalar $(C_1 - 1)$ and identification with (42) shows that we should have

$$R = \frac{1}{\rho_1} - \frac{1}{(1 - C_1)\, S}$$

or taking into account that the reciprocity theory entails :

$$S = 2\, r_1\, \Sigma_1$$

$$R = \frac{P_1 + P_1 P_2(1 + C_1) + P_1 P_2 P_3(1 + C_1 + C_1^2) + \ldots}{P_o(1 + C_1 P_1 + C_1^2 P_1 P_2 + \ldots)(1 + P_1 + P_1 P_2 + \ldots)} \qquad (50)$$

Expressions (49) and (50) are equivalent only for C_1 very near unity and it has been verified that the method of Amouyal and Benoist gives better results, for a non thermalizing fuel region, that the Spectrox method.

In fact equation (41a) can be more generally written as

$$\Sigma_1 V_1 \Phi_1 = P^{o}_{1,1}(\varkappa_1)\, \varkappa_1 V_1 + P'_{b,1} J_1^- \qquad (51)$$

where $P_{1,1}(\varkappa_1)$ is the self-shielding probability for a neutron emitted with the true spatial distribution of $\varkappa_1(r)$.

When the fuel is not thermalizing, it suffices to calculate $P^{o}_{1,1}\ (\phi^{d}_{1})$, the self-collision probability for a neutron emitted with the spatial distribution found by diffusion theory. The ABH method provides, implicitly, another way of evaluating $P^{o}_{1,1}$. Indeed expression (46) is equivalent to evaluating $P^{o}_{1,1}$ in equation (44) by :

$$P^{o}_{1,1} = P_c - (\alpha_1 + \alpha_2 C_1) \left[P_c(1 - C_1) - r_1 \Sigma_{a,1} \cdot (1 - P_c) \right] \quad (52)$$

If the thermalization process doesn't alter too much the spatial distribution of emitted neutrons , expression (52) can still be used and provides a mean of generalizing the AbH method to cases where the fuel region is moderately thermalizing.

The only difference between the ABH and Spectrox formalisms is the particular form of equation (a) of the system (41). In both methods J_1 and J_1^- can be eliminated and the fundamental system to be solved is the made up of four equations in Φ_1 , Φ_M , q_1 and q_M , the two equations resulting from system (41) and the two equations of thermalization (37).

For a non thermalizing.fuel region the method of Amouyal and Benoist gives rapidly the flux structure at each energy :

$$\frac{\Phi_M}{\Phi_1} = 1 + \left[r_1 \Sigma_{a,1} + \frac{\Sigma_{a,1}}{\Sigma_1} A \left(1 + \alpha_1 C_1 + \alpha_2 C_1^2 \right) \right]$$

$$+ \frac{1}{2} r_1^2 \frac{\Sigma_{a,1}}{D_M} h - \frac{3}{2} \frac{r_1^2}{r_2} \Sigma_{a,1} \Gamma \quad (53)$$

One has then

$$V_M L_M \Phi_M = V_M \frac{dq_M}{dE} = \Sigma_{a,1} V_1 \Phi_1 + \Sigma_{a,M} V_M \Phi_M$$

$$= \Sigma'_{a,M} \Phi_M V_M \qquad (56)$$

With the help of the effective absorption cross section $\Sigma'_{a,M}$, the system can be treated as a homogeneous one for the purpose of the treatment of thermalization and all the methods considered in section 2 are applicable.

In the Spectrox method the system of equations to be solved is :

$$\frac{dq_M}{dE} = \Sigma_{a,M} \Phi_M + \frac{\pi r_1}{2 V_M} \frac{1}{R - X} (\Phi_M - \Phi_1)$$

$$= g_{M,M} \Phi_M + g_{M,1} \Phi_1 \qquad (a)$$

$$\frac{dq_1}{dE} = \Sigma_{a,1} \Phi_1 - \frac{\pi r_1}{2 V_1} \frac{1}{R - X} (\Phi_M - \Phi_1)$$

$$= g_{1,1} \Phi_1 + g_{1,M} \Phi_M \qquad (b)$$

(55)

$$\frac{d}{dE}\left(\frac{\Phi_1}{M_1}\right) = J_1 q_1 - \frac{d}{dE}\left(k_1 \frac{dq_1}{dE}\right) \qquad (c)$$

$$\frac{d}{dE}\left(\frac{\Phi_M}{M_M}\right) = J_M q_M - \frac{d}{dE}\left(k_M \frac{dq_M}{dE}\right) \qquad (d)$$

Leslie [4] proposed a very fast finite difference scheme for the solution of (55) with the primary model of thermalization, i.e., $k_1 = k_2 \equiv 0$. With the secondary model one could still use a similar scheme. Inserting expression (a) and (b) for q_1' into equations (c) and (d), and defining the new variables :

$$U_i = B_{i,1}\,\Phi_1 + B_{i,M}\,\Phi_M \qquad i = 1 \text{ and } M \qquad (56)$$

with

$$B_{i,j} = \delta_{i,j} + H_i \frac{\sigma_{i,j}}{(\xi\,\Sigma_s)_i}$$

one has then to solve the system :

$$\frac{dq_i}{dE} = G_{i,1}\,U_1 + G_{i,M}\,U_M$$

$$i = 1 \text{ and } M \qquad (57)$$

$$\frac{d}{dE}\left(\frac{U_i}{M_i}\right) = J_i\,q_i$$

which is formally similar to that solved by Leslie and which is amenable to the same technique of solution.

3.2.3. Extension to cladded fuel elements - The four regions cell [15].

The formalism developped in the previous section is only applicable when the optical thickness of the cladding is very small. Most power reactor fuel elements are canned with stainless steel or zircalloy and the probability of absorption or diffusion in the cladding cannot be ignored. The method of Amouyal and Benoist can easily be extended to such cases.

Let us consider a cell consisting of four successive regions, fuel, can, gap filled with a non-absorbing gas and moderator, indexed 1, 2, 3 and 4 respectively. The possible additional gap between the fuel and the can will be ignored and homogenized with the fuel or the can.

Generally the can does not possess thermalizing properties and the system of equations describing the flux in the cell (equations (28), (29) , (30) , (36) and (37)) can now be written :

$$\Sigma_1 V_1 \Phi_1 = P^o_{1,1} V_1 (\Sigma_{s,1} \Phi_1 + q'_1) + P^o_{2,1} V_2 \Sigma_{s,2} \Phi_2 + P_{b,1} J_3^- \quad (a)$$

$$\Sigma_2 V_2 \Phi_2 = P^o_{1,2} V_1 (\Sigma_{s,1} \Phi_1 + q'_1) + P^o_{2,2} V_2 \Sigma_{s,2} \Phi_2 - P_{b,2} J_3^- \quad (b)$$

$$V_M q'_M = \Sigma_{a,M} V_M \Phi_M + J_3 \quad (c)$$

$$V_1 q'_1 = \Sigma_{a,1} V_1 \Phi_1 + \Sigma_{a,2} V_2 \Phi_2 - J_3 \quad (58) \quad (d)$$

$$J_3^- = \frac{\pi}{2} r_3 \Phi_M + X' J_3 \quad (e)$$

$$\left(\frac{\Phi_1}{M_1} \right)' = j_1 q_1 - (k_1 q'_1)' \quad (f)$$

$$\left(\frac{\Phi_M}{M_M} \right)' = j_M q_M - (k_M q'_M)' \quad (g)$$

We have seen that the ABH method can be considered as consisting of the system of equation (41) with the particular choice of expressio (52) for $P^o_{1,1}$. The generalization of this method to a four region cell will thus be to choose the same expression for the probability $P^o_{1,1}$ appearing in the first equation (58). We shall consider below how to evaluate the other probabilities.

Bonalumi has developped a very fast and accurate calculation procedure for the probabilities $P^o_{i,j}$ in annular systems. Jonsson has further improved this procedure and his method is briefly reviewed in section 3.3. for the general case. For a two regions system whe the flat flux approximation can be applied in each region, its reduces to the following scheme :

$$P^o_{1,1} = P_c(\Sigma_1\ r_1) \qquad (a)$$

$$P^o_{1,2} = (1 - P^o_{1,1})\ G_{1,2} \qquad (b)$$

$$P^o_{2,1} = \frac{\Sigma_1\ V_1}{\Sigma_2\ V_2}\ P^o_{1,2} \qquad (c) \qquad (59)$$

$$P^o_{2,2} = P_c(r_e\ \Sigma_2) - P^o_{2,1}\ G_{1,2} \qquad (d)$$

$$P_{b,i} = \frac{4\ V_i\ \Sigma_i}{S_3}\left(1 - P^o_{i,1} - P^o_{i,2}\right) \quad i = 1,2 \qquad (e)$$

where r_e and $G_{1,2}$ are quantities which will be defined in the next section.

We have seen that, for a three regions cell, the ABH method can be considered as resulting from the particular choice of expression (52) for the probability $P^{o}_{1,1}$ appearing in (41a). The generalization of the ABH method to a four regions cell will thus be to choose the same expression (52) for $P^{o}_{1,1}$ in equation (58a). As the probability $P^{o}_{1,2}$ depends on the distribution of emitted neutron in region 1, expression (52) should also be used for the evaluation of the probability $P^{o}_{1,1}$ appearing in (59b). The probability $C_{1,2}$ has been deduced (see § 3.3.) under the assumption of uniform emission in region 1 but this is not thought to produce an appreciable error as it influences only the angular distribution of neutron entering region 2. All other probabilities ($P^{o}_{2,1}$, $P^{o}_{2,2}$, $P_{b,1}$, $P_{b,2}$) have to be evaluated by equation (59) where $P^{o}_{1,1}$ and $P^{o}_{1,2}$ have evaluated under the flat flux approximations (equations (59a) and (59b)).

All the coefficients of system (58) are now available. If the fuel does not thermalize, which is very often the case, the flux fine structure can easily be evaluated at each energy using equations (a) , (b) , (d) and (e) of the system (58). An effective absorption cross section can then be defined by

$$\Sigma'_a(E) = \Sigma_{a,M} + \frac{V_1}{V_M}\frac{\Phi_1}{\Phi_M}\Sigma_{a,1} + \frac{V_2}{V_M}\frac{\Phi_2}{\Phi_M}\Sigma_{a,2} \qquad (60)$$

and the energy variation of the flux in the moderator region can be evaluated by the techniques developed for homogeneous systems and to be applied now to the set of equations

$$\frac{dq_M}{dE} = \Sigma'_a V_M \Phi_M \qquad (61)$$

$$\frac{d}{dE}\left(\frac{\Phi_M}{M_M}\right) = j_M\, q_M - \frac{d}{dE}\left[k_M \frac{dq_M}{dE}\right] \qquad (61)$$

If the slowing-down density in the fuel is significant, the procedu is more complex. The quantities Φ_2 , J_3 and J_3^- can be eliminated a the set of remaining equations written :

$$\left.\begin{aligned} a_{i,1}\, q_1' + a_{i,2}\, q_2' &= b_{i,1}\, \Phi_1 + b_{i,2}\, \Phi_2 \\ \left(\frac{\Phi_i}{M_i}\right)' &= j_i\, q_i - (k_i\, q_1')' \end{aligned}\right\} \quad i = 1 \text{ and } M \qquad (62)$$

The system formed by the first two equations can be transformed int

$$q_1' = g_{i,1}\, \Phi_1 + g_{i,M}\, \Phi_M \qquad i = 1 \text{ and } M$$

The rest of the calculation proceeds then as for the system (55) in section 3.3.2.

3.3. TREATMENT OF HETEROGENEITY WITH ISOTROPIC BOUNDARY FLUX.

3.3.1. Evaluation of the collision probabilities.

The methods outlined in the preceding sections are based on the use of diffusion theory in the outermost region of the cell. In some cases this region is so thin that this application is not warranted although the ABH method seems to give acceptable results even in tightly packed water moderated lattices [10] .

As indicated previously the system of equations (6) provides an alternative way of evaluating the spatial distribution of the flux, which doesn't rest of the existence of a (relatively) large and weakly absorbing outermost region, provided that one can easily and accurately determine the probabilities $P_{i,k}$.

It seems justifiable to determine the collision probabilities $P^{o}_{i,k}$ for the unit cell with a circularized outer boundary and in one dimensional geometry. Then, the method of Bonalumi [16] , improved by Jonsson [17] , provides an accurate and fast means of determining these probabilities. The first step is of course the determination of $P_{1,1}(\Sigma_1 r_1)$ and this is done with the help of fitting formulae to the tabulation of P_c by Case [14] .

The probabilities $P^{o}_{1,j}$ are obtained through recurrence formulae

$$P_{1,j} = \left(1 - \sum_{k=1}^{j-1} P^{o}_{1,k} \right) G_{1,j} \tag{63}$$

where $G_{i,j}$ is the probability that a neutron entering zone j by its inner boundary with an angular distribution corresponding to uniform birth inside $r_i \leq r_{j-1}$ will collide in zone j. The probabilities $P_{j,1}$ are then obtained through the reciprocity relation (4). $G_{i,j}$ is obtained by the computational scheme

$$\left.\begin{aligned} G_{i,j} &= 1 - \exp(-y_{i,j}) \\ y_{i,j} &= \Sigma_j r_j \tau(x_{ij}) \frac{\pi}{4} \left\{ T\left(\frac{r_i}{r_j}\right) - \alpha_j T\left(\frac{r_i}{r_{j-1}}\right) \right\} \\ \alpha_j &= \frac{r_{j-1}}{r_j} \end{aligned}\right\} \tag{64}$$

$$\left.\begin{aligned} T(u) &= \frac{2}{\pi}\left(\frac{1}{u}\arcsin u + \sqrt{1-u^2}\right) \\ x_{ij} &= \sum_{k=i+1}^{j}\left(r_k - r_{k-1}\right)\Sigma_k - \frac{1}{2}\left(r_j - r_{j-1}\right)\Sigma_j \end{aligned}\right\} \quad (64)$$

τ is a slowly varying function given by Jonsson.

The self-collision probability $P^o_{i,i}$ is given by

$$P^o_{i,i} = P_c\left(r_{i,e}\,\Sigma_i\right) - \left(\sum_{k=1}^{i-1} P^o_{i,k}\right) G_{i-1,i} \quad (65)$$

where the effective radius $r_{i,e}$ can be evaluated according to Schaefer's prescription (see [17]) :

$$\left.\begin{aligned} r_{i,e} &= p(\Sigma_i)\, r_{i,w} + \left(1 - p(\Sigma_i)\right) r_{i,b} \\ r_{i,b} &= r_i(1-\alpha_i^2) \\ r_{i,w} &= r_i\,\frac{1 + \alpha_i^2 - \alpha_i^2\left[E(\alpha_i) + B(\alpha_i)\right]}{1-\alpha_i} \\ p(\Sigma_i) &= \frac{1}{1 + 3\,\Sigma_i\, r_{i,w}} \end{aligned}\right\} \quad (66)$$

where E and B are complete elliptic functions , in fact the factor of r_i in $r_{i,w}$ is given by a fitting formulae. For thick annuli th effective radius reduces to the black radius $r_{i,b}$.

The probability $P^{o}_{i,j}$ $(j > i)$ is made up of two contributions : the first one comes from neutrons entering regions interior to zone i before colliding in zone j, and the second one comes from neutrons leaving zone i outwards. Letting $P^{*}_{i,i-1}$ be the probability that a neutron born in zone i crosses its inner boundary, the first contribution is :

$$\left(P^{*}_{i,i-1} - \sum_{k=1}^{i-1} P^{o}_{i,k} \right)\left(1 - G_{i-1,i} \right) \cdots \left(1 - G_{i-1,j-1} \right) G_{i-1,j} \tag{67}$$

with

$$P^{*}_{i,i-1} = \frac{\pi r_{i-1}}{2 V_i \Sigma_i} G_{i-1,i} \tag{68}$$

The second contribution to $P^{o}_{i,j}$ is given by :

$$\left(1 - P_{i,i-1} - P'_{i,i} \right) \cdots G_{i,j}$$

$$+ \frac{T_i}{1 - \alpha_i^2} \left[\cdots \left(1 - G_{i,j-1} \right) G_{i,j} - \cdots \left(1 - G_{i-1,j-1} \right) G_{i-1,j} \right] \tag{69}$$

with

$$T_i = \alpha_i^2 Q_i \left(1 - G_{i-1,i} \right) + \left(1 - \alpha_i^2 \right)\left(P^{*}_{i,i-1} - \tilde{P}_i \right)\left(1 - G_{i-1,i} \right)$$

$$Q_i = 1 - P_c\left(\Sigma_i \, r_{i-1} \right) \tag{70}$$

$$\tilde{P}_i = \frac{\alpha_i^2}{1 - \alpha_i^2} \, Q_i \, G_{i-1,i}$$

$p'_{i,i}$ is the self-collision probability in zone i without crossing inner regions and is given by :

$$P'_{i,i} = P_c\left(\Sigma_i \, r_{i,e} \right) - P^*_{i,i-1} \, G_{i-1,i} \tag{71}$$

The evaluation of the collision probabilities $P^o_{i,j}$ is terminated by that of $P^o_{i,j}$ for $i > j$ through the reciprocity relation (4). One then proceeds to the evaluation of the effective collision probabilities $P_{i,j}$. In the approximation of isotropic boundary flux, the condition imposed at the outer boundary of the cell is that all neutrons emitted in the cell and reaching its boundary without collisi are compensated by an equal number of neutrons crossing the boundar inwards and with an isotropic angular distribution. P^o_k is the probability that a neutron emitted in region k will reach the boundary without collision.

$$P^o_k = \sum_{i=1}^{N} P^o_{k,i}$$

$P_{b,i}$ is the probability that a neutron crossing the outer boundary inwards will make a collision in zone i of the cell. One has then

$$P_{i,j} = P^{o}_{i,j} + \frac{1 - P^{o}_{j}}{\sum_{k=1}^{N} P_{b,k}} P_{b,j} \qquad (72)$$

Under the assumption of isotropic angular distribution, $P_{b,j}$ is given by

$$P_{b,j} = \frac{4V_j}{2 \pi r_N} \Sigma_j \left(1 - P^{o}_{j} \right) \qquad (73)$$

which is a particular from of the reciprocity relation [14] .

If one does not want to circularized the outer boundary of the cell the Dancoff factor can be used in place of the probabilities $P^{o}_{i,N}$.

The Dancoff correction C is in fact the non collision probability in the region between fuel elements for neutron born uniformly inside one fuel element (regions 1 to N-1). Nothing would be changed in the following section once the effective collision probabilities are determined.

3.3.2. Determination of the fluxes.

The fluxes are determined by the equations (6) of neutrons transport and the N equations (37) of neutron thermalization, i.e. :

$$\left.\begin{aligned} \Sigma_j V_j \phi_j &= \sum_{i=1}^{N} P_{i,j} \left(\Sigma_{s,i} \phi_i + \frac{dq_i}{dE} \right) V_i \\ \frac{d}{dE} \left(\frac{\phi_j}{M_j} \right) &= \lambda_j q_j - \frac{d}{dE} \left(k_j \frac{dq_j}{dE} \right) \end{aligned} \right\} j = 1,N \qquad (74)$$

The set of transport equations can be written in a matrix form :

$$[\ A\ ]\ [\ \Phi\ ] = [\ B\ ]\ [\ q'\ ]$$

where A and B are square matrices. This system can be solved for q' yielding :

$$[\ q'\ ] = [\ C\ ] \cdot [\ \Phi\ ]$$

with

$$[\ C\ ] = [\ B\ ]^{-1} \cdot [\ A\ ]$$

The slowing-down densities can now be eliminated from the thermalization equations, through the introduction of new functions :

$$U_i = \sum_{j=1}^{N} D_{i,j}\ \Phi_j \qquad (76)$$

with

$$D_{i,j} = \delta_{i,j} + \frac{H_i}{(\xi\ \Sigma_s)_i}\ g_{i,j}$$

One then gets :

$$\frac{d}{dE}\left(\frac{U_i}{M_i}\right) = J_i\ q_i$$

or

$$(\xi\,\Sigma_{s,i})\,\frac{d}{dE}\left\{\frac{1}{G_i}\left[\,KT\,\frac{dU_i}{dt}+\left(E-KT\right)U_i\,\right]\right\}$$

$$=\sum_{j=1}^{M} C^{*}_{i,j}\,U_j \qquad\qquad i=1,M \qquad\qquad (77)$$

with $[\,C^{*}\,]=[\,C\,]\cdot[\,D\,]^{-1}$

The system of equation (77) is amenable to the same technique of solution as the set of equations solved by the Spectrox method. When M is larger than 2, some generalization of the Spectrox scheme would be required. These techniques are only interesting when the number of regions is small, which is normally the case with collision probability methods.

On the other hand particular attention should be paid to regions where the slowing-down densities are small or where one wishes to ignore them (metallic fuel, cladding, etc). In many cases an iterative procedure would be preferred.

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* *

4.- ASSESSEMENT OF THE FORMALISM.

4.1. SCOPE OF THE ASSESSEMENT.

The ultimate justification of the formalism described above will be achieved by the comparison of the predicted neutron fluxes with either very fine experimental results on the prediction of the most elaborate procedures, such as two-dimensional DSN calculations. In the meantime we can assess separately some steps in the computational scheme, in order to have a reasonable a priori confidence in this scheme.

4.2. GENERAL COMPARISON WITH OTHER CODES.

The results of the THERMOS code [10] are at present widely used as a convenient reference for other methods. For this reason it is instructive to list the differences between this code and the computational schemes proposed here. The main differences are :

- the use of the synthetic model of thermalization instead of differential transfer cross sections,
- the use of the method of Bonalumi - Jonsson for the evaluation of collision probabilities,
- a different treatment of the outermost region of the cell, that is assymptotic diffusion theory when this region is large and weakly absorbing and in other cases, effective collision probabilities based on either its Dancoff correction on the approximation of isotropic boundary flux.

All these points have already been discussed quite thoroughly. In particula it has been found that the ABH method gives good results even for tightly packed water moderated lattices [10] , that the method of Bonalumi - Jonsso allows the evaluation of collision probabilities with sufficient accuracy [15] , [17] and that the secondary model of thermalization is a good substitude for multigroup methods for usual moderators [3] ,[19].

In the following sections we shallonly investigate further the suitability of the thermalization model. It has been shown that by a proper adjustment of the functions j(E) and k(E) (or G and H), the results of this model can be made to agree closely with those of multigroup methods with a large number of groups [19] . More specifically, for homogeneous system moderated with light or heavy water, the agreement on the fluxes is within a few percents, and that on the effective cross-section within a fraction of one percent up to the following absorption rates :

$$\frac{\Sigma_a(2200)}{\xi \Sigma_s} = 2 \qquad \text{for 1/v absorption,}$$

$$\frac{\Sigma_a(2200)}{\xi \Sigma_s} = 0.4 \qquad \text{for Pu-239 absorption}$$

A similar comparison for graphite moderated systems had been reported previously [3] .

4.3. NUMERICAL COMPARISON WITH MULTIGROUP METHODS.

4.3.1. Light water moderated systems.

We have done some other comparisons for homogeneous and heterogeneous systems moderated with either light water or graphite. For light water moderated systems, the results of the PANTHER (or BN 172) programme [20] have been checked against those of LASER for the Pu bearing lattices studied at Hanford and Westinghouse ; the following tables are extracted from this evaluation study [21].

Hanford lattices.

Pitch (cm)	K_{eff}(PANTHER)	K_{eff} (LASER).
0.55	0.9924	0.9932
0.60	0.9956	0.9954
0.71	1.0010	0.9990
0.80	0.9997	0.9974
0.90	0.9974	0.9976
0.93	1.0007	0.9961

Westinghouse lattices.

Pitch (cm)	K_{eff}(PANTHER)	K_{eff} (LASER)
0.52	0.9927	0.9961
0.56	1.0089	1.0114
0.735	1.0009	1.0067
0.790	1.0034	1.0094
1.04	1.005	1.0139

For this comparison the plutonium cross-sections were normalized to the 2200 m/s data of Winfrith. The epithermal and fast events ($E > 1.855$ eV) were treated with MUFT.

4.3.2. Graphite moderated systems.

For graphite moderated systems, the results of another programme [22] have been checked with those of the WIMS A code developped at Winfrith. This latter code treats the whole energy range from 0 t 10 MeV and has 44 groups in the thermal region up to 4 eV, with a v ry fine group structure across the plutonium 239 and plutonium 240 thermal resonances at 0.29 and 1.057 eV respectively.

It includes several modes of treatments of cell heterogeneity and in particular DSN and PERSEUS [18] . The latter has been selected for this comparison as the heterogeneity treatment in our programme is based on the same method. The differences in nuclear data being small, the comparison below will clearly indicate the effects of the treatment of thermalization, and only this effect..

The systems investigated in greater details and reported here are all at a temperature of 700 °K and without leakage. To simplify the interpretation of the results, they contain only three isotopes, graphite, plutonium 239 and plutonium 240. They are characterized by the ratio of the overall graphite atomic density to the overall plutonium 239 atomic density and by the percentage of the isotope 240 in the plutonium. The functions G(E) and H(E) for graphite were interpolated from the functions adjusted on Egelstaff's model and supplied by J.L. Soulé.

Two homogeneous systems have been considered, characterized respectively by :

1) C/Pu-239 = 3000 16.66 % of Pu-240

2) C/Pu-239 = 5000 16.00 % of Pu-240

Although these systems are very undermoderated, the secondary model gives excellent results, as can be seen from figures 2 and 3. Only the flux dip due to the plutonium 240 resonance is somewhat underestimated. The success of the method is best demonstrated by comparing the effective thermal cross-sections averaged from 0 to 1.5 eV. Defining :

$$\Delta \bar{\sigma}_a = \left(\bar{\sigma}_a(SM) - \bar{\sigma}_a(WIMS) \right) \Big/ \bar{\sigma}_a(WIMS)$$

one has for the harder spectrum (C/Pu-239 = 3000)

$\Delta \bar{\sigma}_{a,Pu-239} = + 0.1$ %

$\Delta \bar{\sigma}_{a,Pu-240} = + 1.5$ %

One heterogeneous system has also been considered. The specification of the two-regions cell of the infinite lattice have been chosen so as to give simultaneously a significant spatial shielding of the Pu resonances and a large amount of thermalization in the central fuelled region. These specifications are :

	Region 1	Region 2
External radius (cm)	3.9	6.4
Volume fraction	0.37134	0.62866
N_C (10^{24} at/cm^3)	0.085	0.088
N_{Pu-239} (10^{24} at/cm^3)	0.078 10^{-3}	0.0
N_{Pu-240} (10^{24} at/cm^3)	0.01486 10^{-3}	0.0

One has also :

C/Pu-239 = 3000 16 % of Pu-240

Here about one third of the thermalization occurs in the fuelled region, in opposition with most systems studied so far with the synthetic model where the fuel region was only weakly thermalizing The interest of this case is therefore to provide a stringent test of the adequacy of the synthetic model of thermalization for the evaluation of the flux variation across the cell. As can be seen from figure 4 this test is conclusive. Again, the flux dip due to the Pu-239 resonance is very accurately predicted, while the dip d to the Pu-240 resonance is somewhat underestimated ; the averaged thermal cross-sections are also in good agreement.

Obviously the lay-out of the unit cell is not realistic and the flux variation across the cell is too large to be amenable to a simple first collision probability treatment with two zones ; a WIMS case where the central region is divided in seven zones and the outer region in three zones gives ϕ_1/ϕ_2 ratios significantly larger than previously, especially at resonance peaks. This fact, however, doesn't alter the conclusions relative to the applicability of Cadilhac's model of thermalization.

*

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5.- CONCLUSIONS.

It has been demonstrated that there is no difficulty at all in linking the synthetic model of neutron thermalization proposed by M. Cadilhac with the treatment of cell heterogeneity by various collision probability methods. The resulting equations can easily be solved on a modern computer with a significant gain of time compared with accurate multigroup methods. Comparison of these different approaches has been performed for plutonium fuelled light water and graphite moderated systems. The examined graphite cases have the advantage to provide a more stringent check of the synthetic model (scattering law, resonance absorption, thermalization in the fuel). Besides confirming that the Cadilhac's model is excellent for homogeneous systems, it was found that the flux distribution across the cell is very accurately predicted in heterogeneous systems, even when there is a significant amount of thermalization in regions containing resonance absorbers. There is no doubt that the proposed computational schemes are very valuable tools for the survey of plutonium fuelled light water moderated lattices and fuel depletion studies in water reactors.

*

* *

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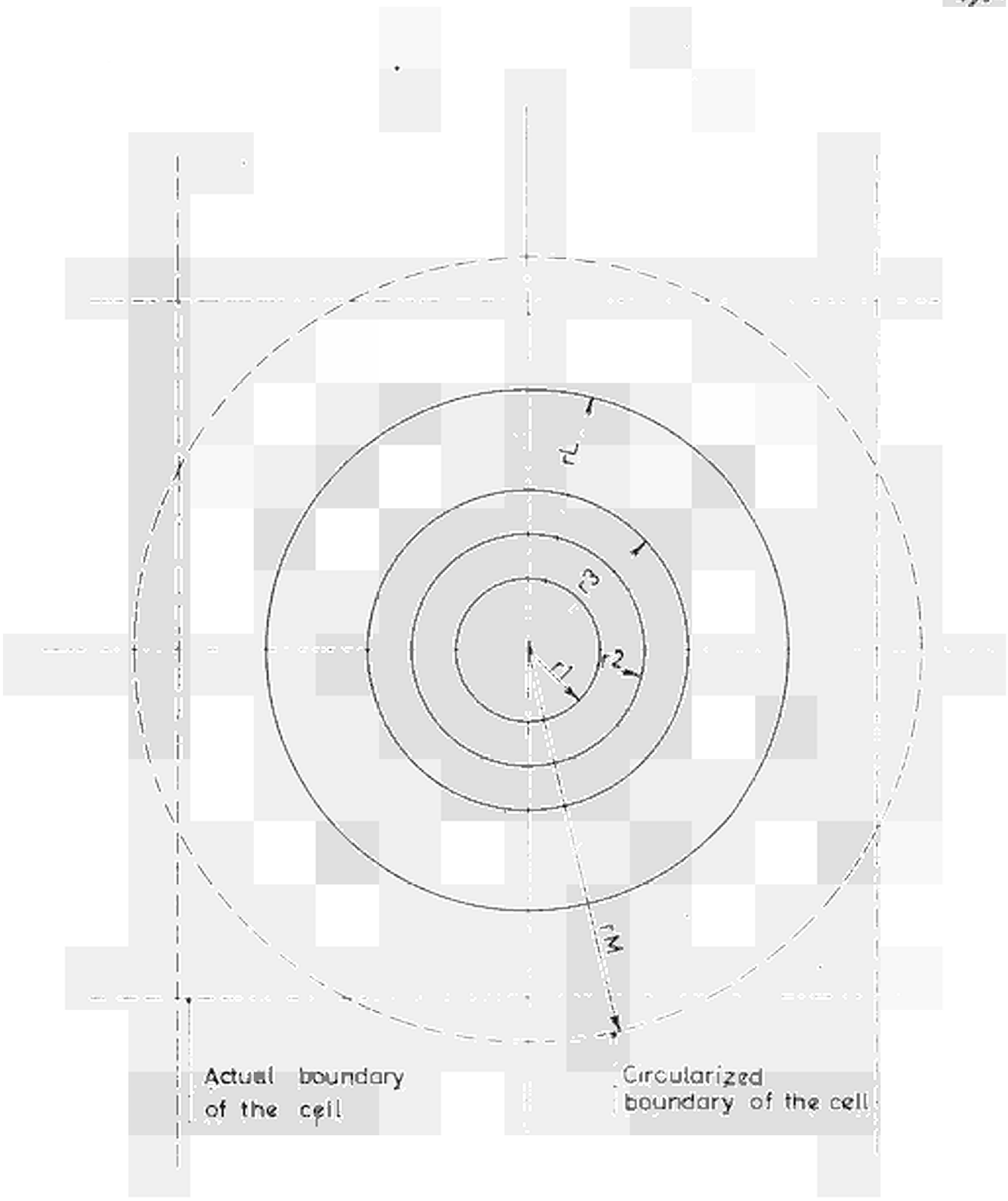


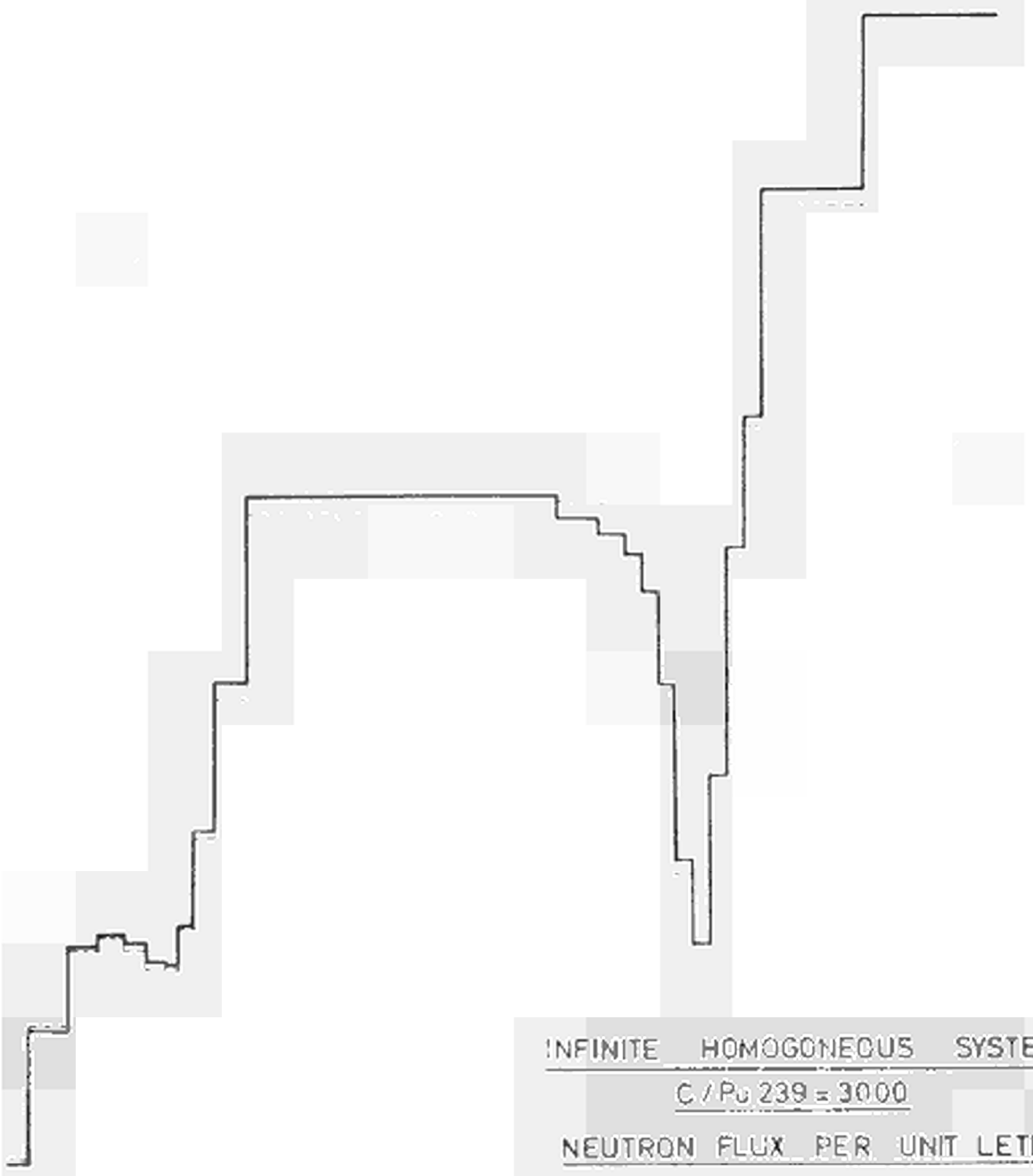
DESIGN OF THE UNIT CELL

FIG. 1

Condensed from a 38 groups spectrum from 0 to 1.5 eV predicted by WIMS A

Secondary model _ Spectrum condensed into the same group structure as above

u

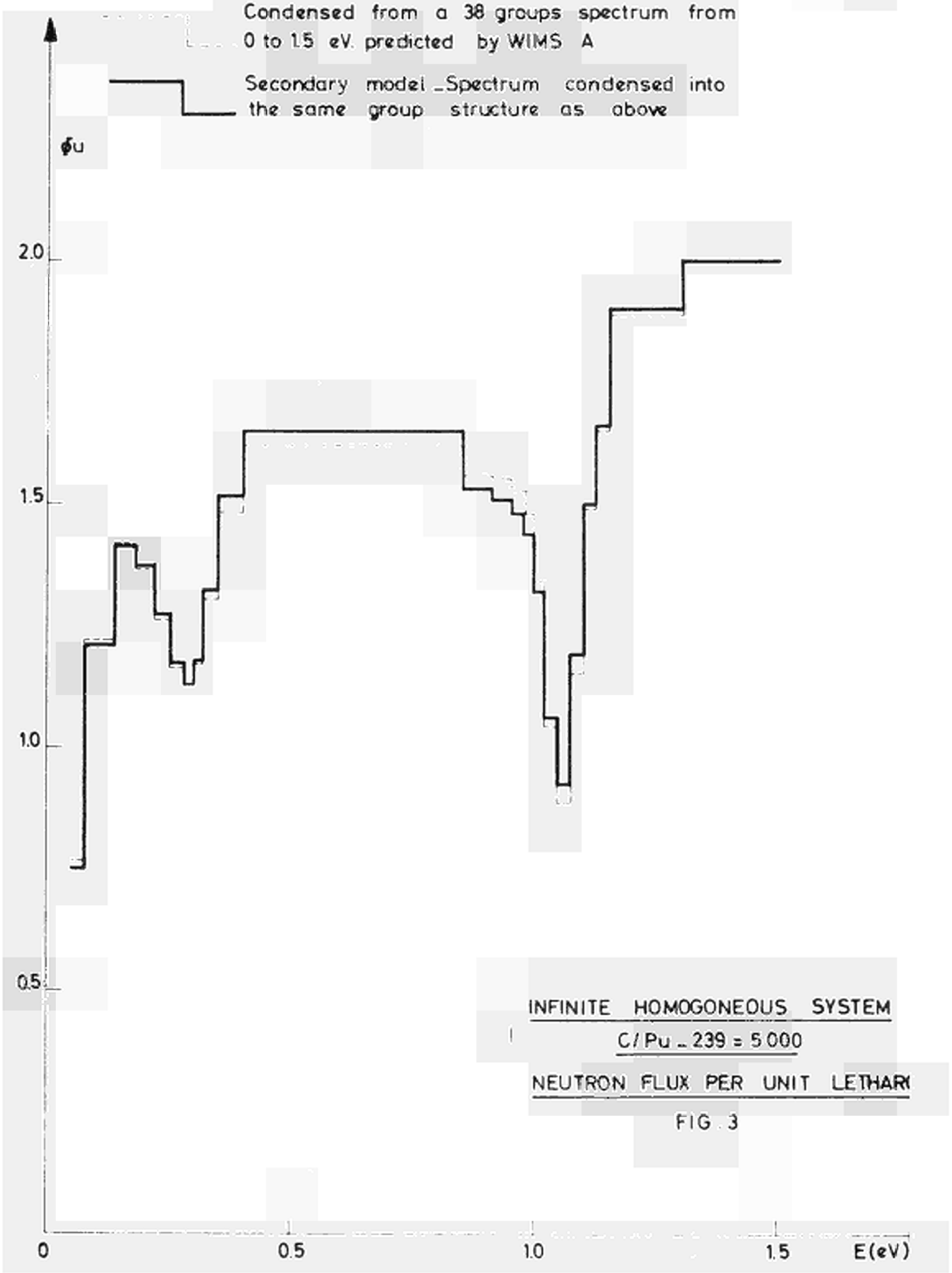


INFINITE HOMOGONEOUS SYSTEM

C / Pu 239 = 3000

NEUTRON FLUX PER UNIT LETHARGY

FIG. 2



INFINITE HOMOGONEOUS SYSTEM

C/Pu _ 239 = 5 000

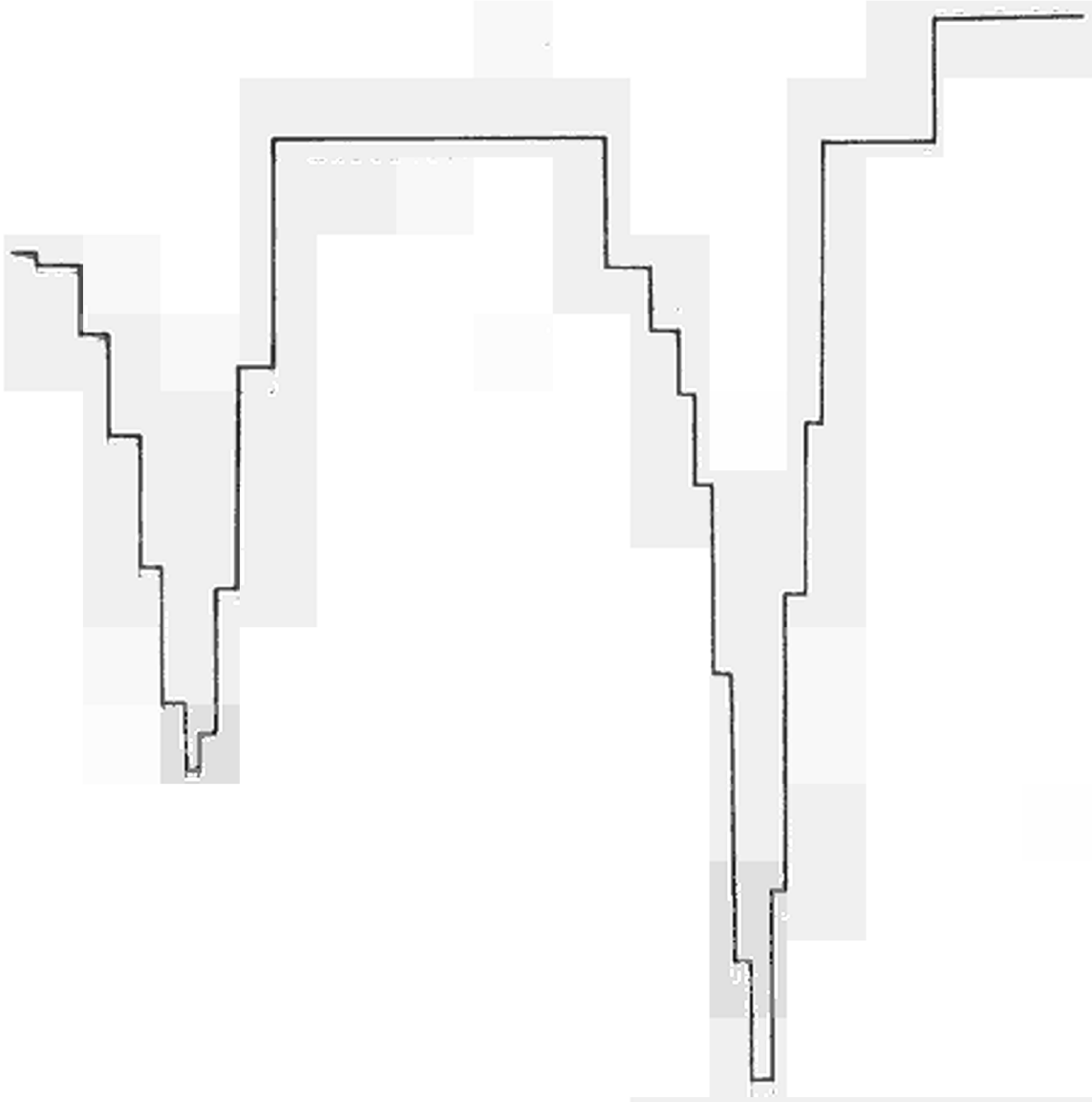
NEUTRON FLUX PER UNIT LETHARG

FIG. 3

WIMS A Ratio of the condensed fluxes

Secondary model Ratio of the condensed fluxes

$\frac{\phi 1}{\phi 2}$



INFINITE HETEROGENEOUS SYSTEM

C/Pu 239 = 3.000

RATIO OF THE FLUX IN THE INNER REGION

TO THE FLUX IN THE OUTER REGION

FIG. 4

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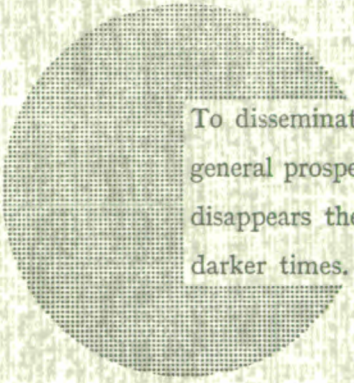

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Alfred Nobel

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